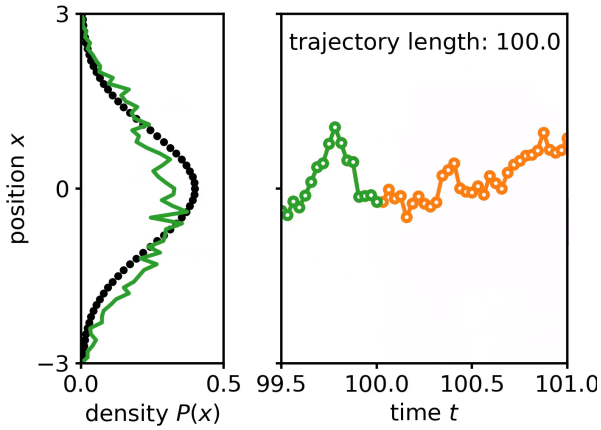
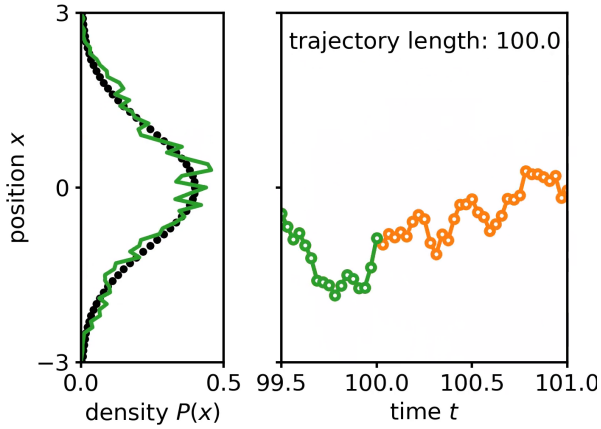
Path-accelerated stochastic molecular dynamics: Parallel-in-time integration using path integrals

Supplementary movie captions



Supplementary movie M1. At right, animation of a PAMD simulation, using the same parameters as for the $N_{\text{sample}} = 1$ case of Fig. 3E in the main text. The color scheme in this panel follows that of Fig. 2, with the last portion of the resolved trajectory shown in green and with the sampled path shown in orange. The time axis indicates the elapsing MD simulation time. At left, the cummulative histogram of sampled positions in the resolved trajectory (green line), relative to the analytical result (black dots). As seen in Fig. 3E, the resulting distribution sampled by the path-accelerated dynamics is not accurate using this set of parameters.



Supplementary movie M2. At right, animation of a PAMD simulation, using the same parameters as for the $N_{\text{sample}} = 4$ case of Fig. 3E in the main text. The color scheme in this panel follows that of Fig. 2, with the last portion of the resolved trajectory shown in green and with the sampled path shown in orange. The time axis indicates the elapsing MD simulation time. At left, the cummulative histogram of sampled positions in the resolved trajectory (green line), relative to the analytical result (black dots). As seen in Fig. 3E, the resulting distribution sampled by the path-accelerated dynamics is highly accurate using this set of parameters.